# Appendix A: CSMGem Example Problems

## A.1 Introduction

The Center for Hydrate Research has been conducting hydrate experiments for over 30 years in efforts to improve flow assurance strategies. The first statistical thermodynamic model for hydrates was developed in 1959 and involved many assumptions, including the assumption that volume is constant. This model predicted hydrate formation temperatures and pressures reasonably well at temperatures near the ice point and at low pressures. However, as industry moves to deeper waters, there is a need for a hydrate model that can predict hydrate formation at higher temperatures and pressures.

The new hydrate model relaxes the constant volume assumption. This model, coupled with the models for aqueous, vapor, liquid hydrocarbon, ice, and solid salt phases, is the basis of CSMGem. CSMGem can calculate multiphase equilibria at any given temperature and pressure using an algorithm based on Gibbs energy minimization. CSMGem is tailored specifically to the hydrocarbon industry in that the models used are regressed in temperature and pressure ranges typically found in subsea pipelines (i.e., temperatures above the ice-point and pressures up to 15,000 psia).

Phase equilibria can be calculated for the following conditions:

- Incipient hydrate formation temperature at a fixed pressure
- Incipient hydrate formation pressure at a fixed temperature
- Fixed temperature and pressure
- Fixed temperature and specified phase fraction (i.e., dew and bubble points)
- Fixed pressure and specified phase fraction (i.e., dew and bubble points)
- Expansion through a valve (i.e., fixed pressure and enthalpy)
- Expansion through a turboexpander (i.e., fixed pressure and entropy)

CSMGem can also plot phase boundaries when used in conjunction with MS Excel.

Please see the "Read me" statement on the CD for installing the program. Also note a complete user's guide on the CD.

The authors acknowledge the Center for Hydrate Research Consortium members for the funding and data required for the development of CSMGem. Consortium members include: BP, Chevron, ConocoPhillips, ExxonMobil, Halliburton, Petrobas, Schlumberger, Shell, Statoil.

## A.2 Example Problems

The following example problems are all performed with a given natural gas mixture and will be saved as "Feed.csm." The natural gas selected for the problems has the following composition:

| | |
|---|---|
| Methane | 0.9033 |
| Ethane | 0.0519 |
| Propane | 0.0140 |
| *n*-Butane | 0.0031 |
| *i*-Butane | 0.0022 |
| *n*-Pentane | 0.0005 |
| *i*-Pentane | 0.0007 |
| *n*-Hexane | 0.0002 |
| Nitrogen | 0.0206 |
| Carbon dioxide | 0.0035 |
| Water | 10 mol% of gas mixture |

*Note*: The temperature and pressure of hydrate formation is slightly dependent on the amount of water in the feed. However, this is of more concern when alcohols are present due to partitioning. It is recommended to use approximately 10 mol% of water relative to the gas mixture.

## A.3 Setting up the Natural Gas Example

To perform calculations with the above gas mixture do the following:

1. Open the Components Selection menu, check the above components and then press OK button
2. Feed menu opens automatically. Change the feed units to "mole fraction". Input the above composition with the exception of water (Figure A.1)
3. Click on Aqueous Phase Calculator
4. Input "10" into Amount box for Water and select "mol% Feed + Water"
5. Press OK button
6. Open Units menu and select Fahrenheit and psia for the $T$ and $P$ units, respectively

## A.4 Incipient Hydrate Formation Conditions

The objective next is to determine the hydrate formation pressure at a given temperature (35°F). To perform this calculation, do the following:

1. Open Incipient Hydrate Formation form and select Hydrate Formation $P$ at given $T$
2. Input "35" into Temperature box
3. Press Calculate button

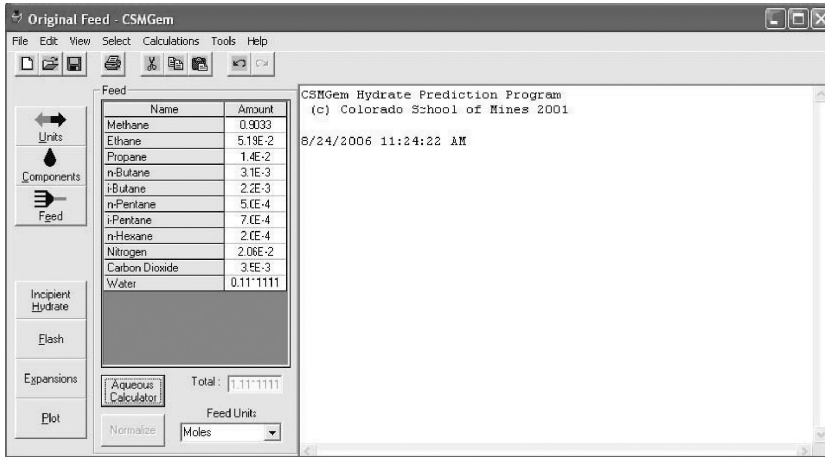


**FIGURE A.1** Layout of feed screen for fluid composition input.

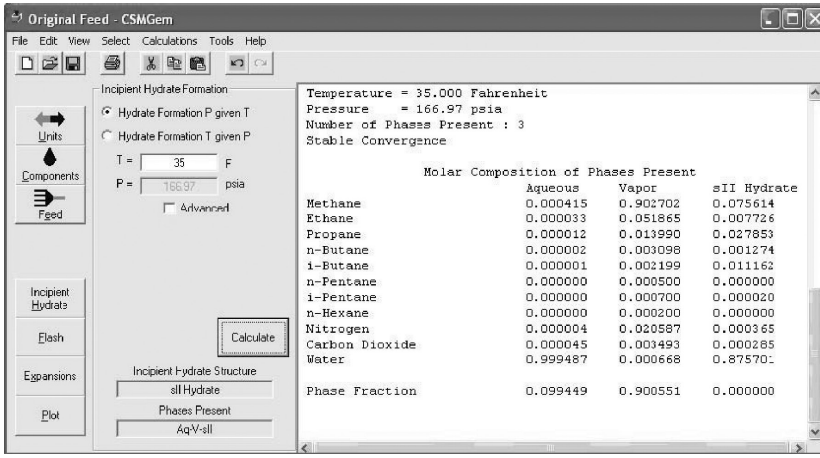


**FIGURE A.2** Layout for "hydrate formation $P$ given $T$" calculation.

CSMGem predicts sII hydrate to form at a pressure of 166.97 psia (Figure A.2). *Note*: If Advanced box is checked, the output for sI and sH hydrates is "$P > P$ sII." This simply means that the calculation was only performed for sII and that it was internally determined that sI and sH were not stable.

The next objective is to determine the hydrate formation temperature at a given pressure (200 psia). To perform this calculation, do the following:

1. Open Incipient Hydrate Formation form and select Hydrate Formation $T$ at given $P$
2. Input "200" into Pressure box
3. Press Calculate button

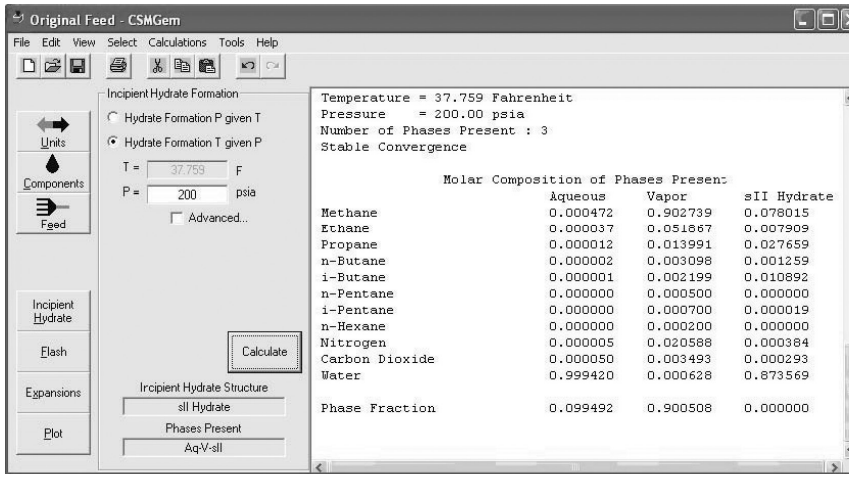


**FIGURE A.3** Layout for "hydrate formation $T$ given $P$" calculation.

CSMGem predicts sII hydrate to form at a temperature of 37.759°F (Figure A.3).
*Note*: If the Advanced box is checked, the output for sI and sH hydrates is "$T < T$ sII." This simply means that the calculation was only performed for sII and that it was internally determined that sI and sH were not stable.

## A.5 PLOTTING A 2-PHASE VLE CURVE

We will create a water-free 2-Phase VLE envelope next. Because the bounds for this calculation are automatically set, we only need to open the Plot form and select the "2-Phase VLE" option and press the Plot button to create the plot:

1. Open Plot form, found in the bottom left corner of the interface
2. Select "2-Phase VLE" option
3. Press Plot button

Depending on the speed of your computer, it may take some time to calculate the envelope and open the plotting tool (especially if you are using MS Excel). The final plot should look like Figure A.4.

## A.6 ADDING HYDRATE INHIBITOR

1. Add methanol (MeOH) to components list
2. Go to "Aqueous Calculator" form under the "Feed" menu
3. Add a mass ratio of 0.1 g methanol/g water (see Figure A.5).

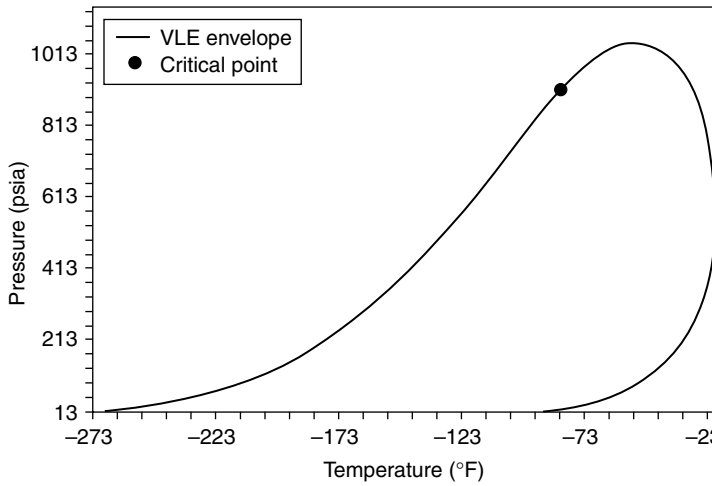


**FIGURE A.4** Output for "2-Phase VLE."

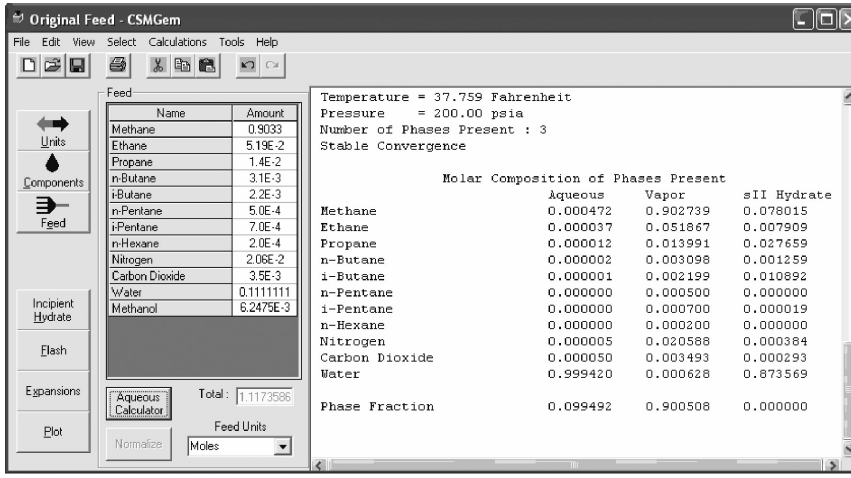


**FIGURE A.5** Components list with methanol concentration at 0.1 g/g water.

What is the new equilibrium pressure at 35°F?
What is the new equilibrium temperature at 200 psia?

4. Increase the methanol concentration to a mass ratio of 0.5 g methanol/g water

What is the new equilibrium pressure at 35°F?
What is the new equilibrium temperature at 200 psia?

## A.7 Adding Hydrate Inhibitor Solutions

Methanol mass ratio of 0.1:

The new equilibrium pressure at 35°F is: 253.67 psia.
The new equilibrium temperature at 200 psia is: 31.383°F.

Methanol mass ratio of 0.5:

The new equilibrium pressure at 35°F is: 2104.1 psia.
The new equilibrium temperature at 200 psia is: 7.78°F.

## A.8 Expansion Across a Valve

Determine the temperature downstream of a choke valve:

1. Click on "Expansions" option
2. Select "Valve"
3. Enter an inlet pressure of 3500 psia and temperature of 65°F (see Figure A.6)
4. Enter an outlet pressure of 3250 psia
5. Check the "initial guess" box and set this to "1F". Press the Calculate button

What is the outlet temperature?
What is the new temperature if the outlet pressure is reduced to 3100 psia?
*Hint*: You may need to use an initial guess to get the iteration to converge (try 50°F).

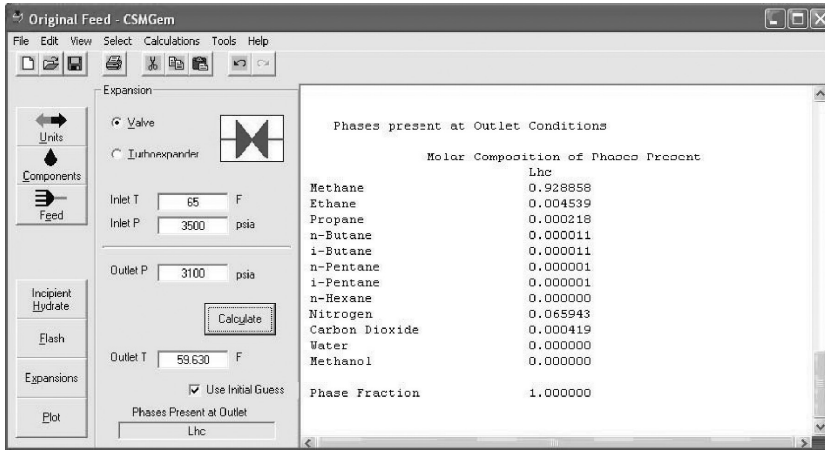


**Figure A.6** Layout for expansion across a valve.

## A.9 Expansion Across a Valve Solutions

Outlet temperature is 61.81°F when the outlet pressure is 3250 psia.
The outlet temperature is 59.63°F when the outlet pressure is 3100 psia.

## A.10 Real Life Situation

Using the initial composition above, answer the following question from a real life situation. Make sure to remove methanol for the first part of the question.

A subsea well head is at 2000 psia and 85°F. A choke valve is to be installed to regulate the downstream pressure:

1. What is the maximum pressure drop that can be sustained without danger of hydrate formation?
2. What is the temperature at this pressure?
3. What is the maximum pressure drop with a 10 wt% (0.1 g/g water) methanol addition?

Isenthalpic expansion and "10 mol% feed + water" can be assumed.

Use the Plot tab on CSMGem to plot the isenthalpic expansion curve using MS Excel. Save this data under a different file name before continuing to plot-phase boundaries. The file will be overwritten if the name is not changed.

Use the Plot tab on CSMGem (add # intervals required) to plot the sII phase boundaries with and without methanol using MS Excel. After combining the calculated data, the final plot should look like Figure A.7. The solutions are the intersection of the expansion line and sII phase boundary lines.

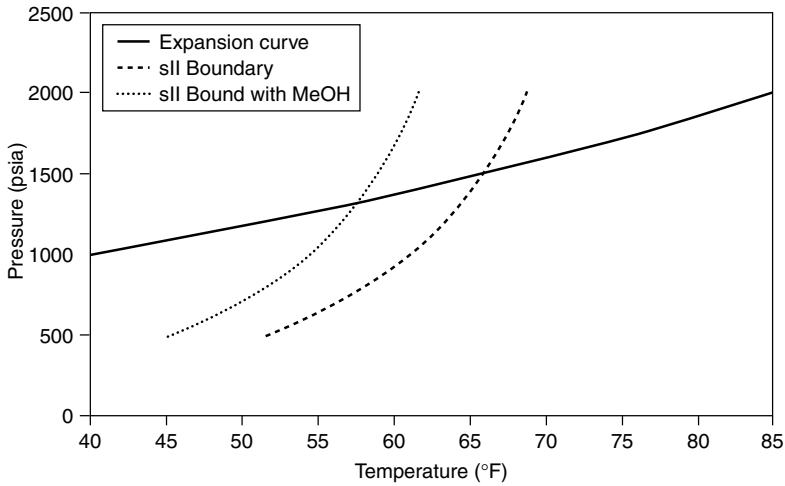


**Figure A.7** Phase diagram for hydrate formation.

Downstream conditions at equilibrium point:

*Without methanol*: Temperature = 66°F; Pressure = 1480 psia.
*With methanol*: Temperature = 57°F; Pressure = 1320 psia.